Lawrence Livermore National Laboratory

Science & Technology Review

July 2020

2019 R&D 100 AWARD WINNERS

Also in this issue:

- **Developing Innovative Hohlraum Designs**
- **Advances in Detecting Dark Matter**
- **Cross-Section Experiment Yields Surprising Results**

About the Cover

Laboratory researchers won four R&D 100 awards in 2019 as part of *R&D World Magazine*'s annual competition for the top 100 industrial innovations worldwide. Highlights beginning on p. 4 describe the award-winning technologies. These winners include a low-density polymer foam plug for occluding blood vessels, a multilevel checkpointing system for improved simulation performance on supercomputers, a faster open-source software package manager, and a novel portable neutron multiplicity detector. Since 1978, Livermore researchers have received more than 160 R&D 100 awards. The R&D 100 logo is reprinted in this issue with permission from *R&D World Magazine*.

Cover design: Mary J. Gines

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Many of the articles in this issue were written prior to the onset of the COVID-19 pandemic. The Laboratory is now actively engaged in the national effort to mitigate COVID-19 and address its effects. Visit www.llnl.gov/coronavirus for up-to-date information on Livermore's COVID-19 research, and stay tuned for future issues of S&TR that will include articles on this topic.

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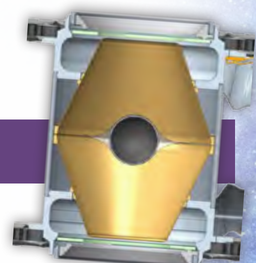
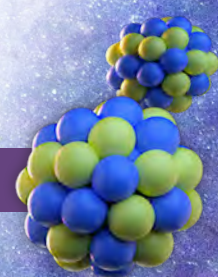


Research Highlights

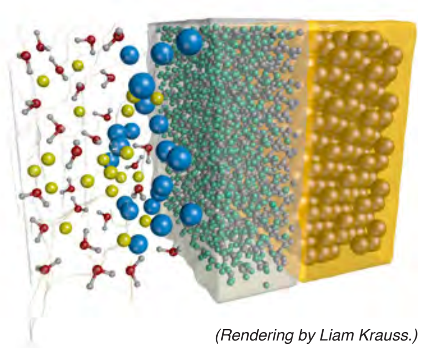


Departments

Exploring Ion Transport in Nanoporous Materials

Understanding and controlling the movement of ions in porous materials and at hydrophobic interfaces is critical to a wide variety of energy and environmental technologies. However, a detailed understanding of how such transport occurs at the nanoscale is still in its infancy. In a recent study, Lawrence Livermore scientists, in collaboration with the University of California at Irvine, demonstrated that ion transport of aqueous solutions at a hydrophobic interface can be highly dependent on the size and hydration strength of the solvated ions. The team's results appeared in the March 17, 2020, issue of *ACS Nano*.

As part of the research effort, the team designed nanopores containing a hydrophobic entrance on one side and a hydrophilic, highly charged entrance on the other side. During experiments, this configuration allowed the researchers to induce the wetting of nanopores using lower voltages (less than 2 volts) and explore gating—ion activation and deactivation—with different ion types. The team's experimental results, coupled with first-principle calculations and molecular dynamics simulations, revealed that large anions, such as bromine and iodine, are prone to migrate from an aqueous solution to a hydrophobic interface. (See image above.) This process leads to the anion accumulation responsible for pore wetting and enhanced ion currents.



(Rendering by Liam Krauss.)

Lawrence Livermore's Anh Pham, co-author of the research paper, explains, "The findings are important for designing nanoporous systems that are selective to ions of the same charge, as well as for realization of ion-induced wetting in hydrophobic pores." Such systems are relevant in applications ranging from ion-selective membranes, drug delivery platforms, and biosensing to ion batteries and supercapacitors.

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Harvesting Waste Heat from Untapped Sources

In the United States, thirteen quadrillion British Thermal Units (BTUs) of energy—enough to meet the nation's total energy needs for 47 days—are lost annually to waste heat. Recently, a team of materials scientists, led by Livermore's Alex Baker, have developed a cold-spray deposition technique to fabricate cost-efficient thermoelectric generators that can harvest waste heat from previously inaccessible sources. The research appeared in the April 8, 2020, edition of *JOM (Journal of The Minerals, Metals, & Materials Society)*.

In conventional cold-spray deposition, micrometer-scale metal particles are entrained in supersonic gas and directed onto a metal surface. Upon impact, the particles plastically deform and bond with the surface or one another. Typically, this process has been limited to malleable materials, as functional materials, such as thermoelectrics, tend to become brittle. Funded by the Department of Energy's Technology Commercialization Fund Program, Livermore and industrial partner TTEC Thermoelectric Technologies, LLC, used their additive manufacturing technique to cold spray thermoelectric bismuth-telluride powder onto substrates including stainless steel, aluminum silicate, and quartz. After deposition, the material showed no significant compositional change, indicating that thermoelectric generators can be fabricated without loss of integrity.

This process can be used to apply thermoelectric materials in place, creating generators that efficiently harvest waste heat emitted from components with complex shapes, such as pipes and valves. Says Baker, "We demonstrated the power and versatility of cold-spray additive manufacturing to build thermoelectric generators in locations that had been inaccessible with traditional approaches using rigid thermoelectric devices."

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Livermore Supercomputer Supports COVID-19 Research

As COVID-19 began impacting millions of people worldwide, Lawrence Livermore, Penguin Computing, and Advanced Micro Devices, Inc. (AMD), reached an agreement to upgrade the Laboratory's Corona computing cluster with an in-kind contribution of cutting-edge AMD Instinct™ accelerators. "These accelerators boost the capability of the teams working on COVID-19," says Livermore's Jim Brase, the Computing Directorate's deputy associate director for programs. "We can work faster, with more throughput."

Using Corona, a Livermore team implemented a first-of-its-kind virtual screening platform to evaluate therapeutic antibody designs that could improve binding interactions with the antigen protein in SARS-CoV-2 (the virus that causes COVID-19). The team has narrowed the list of antibody candidates from a nearly infinite set to about 20 possibilities and has begun exploring additional antibody designs. The new accelerators allow researchers to increase the number of computationally expensive simulations they can perform, making the discovery of an effective antibody design more likely.

With the system upgrade complete as of April 2020, the Penguin Computing–built Corona machine—named for the total solar eclipse of 2017—exceeds a peak performance of 4.5 petaflops (10^{15} floating-point operations per second). In addition to the work being conducted by Lawrence Livermore researchers on discovery of potential antibodies and antiviral compounds, Corona is being utilized by the COVID-19 HPC Consortium, a nationwide public–private partnership involving more than a dozen member institutions in government, industry, and academia that aims to accelerate development of detection methods and treatments for the virus.

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Commentary by Patricia Falcone

Celebrating a Culture of Innovation

SINCE Lawrence Livermore's founding, the Laboratory has embraced the credo of new ideas to address important problems. Responding to the nation's need for national security science and technology has been a catalyst for creative problem solving that continues today. We are driven by our national security mission, which brings an urgency to our work. Livermore's capabilities and expertise have always evolved to meet these needs, and this philosophy has naturally made its way into other scientific domains. This approach is particularly relevant now as we work with the scientific community to address the COVID-19 pandemic (llnl.gov/coronavirus).

Today—nearly 70 years after the Laboratory's gates opened—our culture of innovation and discovery is very much alive. Over the years, we have produced many award-winning technologies, including more than 160 products, devices, and processes that have garnered recognition from the prestigious R&D 100 Award competition. In 2019, we were honored to have received four of these awards. Our winners are featured in this issue of *Science & Technology Review* beginning on p. 4.

Two of these technologies are software tools that solve different problems in high-performance computing (HPC). The Spack package management tool simplifies and automates deployment of large-scale scientific software applications. Spack's large, centralized repository of package recipes reduces redundancies by leveraging others' work, and the tool's flexibility lets users customize their application builds for any machine. Once a scientific application is running, bottlenecks often occur when simulation data is written to the supercomputer's long-term storage nodes. The Scalable Checkpoint/Restart (SCR) framework eases this burden by exploiting intermediate levels of storage. The application can run more quickly—reducing time to solution—thanks to SCR's accelerated data movement.

A third winner is an advanced material that improves blood vessel embolization. The IMPEDE® embolization plug brings Livermore's materials science capabilities to bear on the medical need to stop uncontrolled blood flow through vessels, such as those damaged by aneurysm leaks, trauma, and other conditions. Working with collaborators in academia and industry, the development team has created an optimized shape-memory-polymer foam that expands to fill and protect a damaged vessel. As part of the research effort, the team also used the Laboratory's HPC systems to simulate blood flow and material strength, demonstrating the range of treatment opportunities to clinicians.

Our fourth winner is a specialized detector that aids in nuclear nonproliferation efforts. The MC-15 portable neutron multiplicity detector zeroes in on neutron multiplication as an indicator of nuclear fission, helping security teams quickly identify the presence of special nuclear materials. Similar to other finely calibrated instrumentation developed at the Laboratory, the MC-15 system is operator-friendly and portable.

While extraordinary scientific and engineering capabilities and talented staff make us a wellspring of creativity, we purposefully work to embrace the practices of "open innovation" by connecting with new partners, embracing novel approaches, and working beyond the Laboratory site. The R&D 100 Award–winning technologies described herein were all carried out with collaborators. We are also fortunate to be situated close to Silicon Valley, where invention and entrepreneurship are a way of life, and the competition is healthy. We find many opportunities for technology transfer in this environment. In addition, our researchers come from many different backgrounds and cultural experiences. This diversity creates a constant exchange of ideas, and we are better for it. On behalf of the Laboratory's leadership team, I offer a hearty congratulations to our 2019 R&D 100 Award winners, who have all successfully demonstrated what a culture of innovation can accomplish.

■ Patricia Falcone is deputy director for Science and Technology.

Portable Threat Assessment

SECURITY teams responding to potential nuclear threats require quick and accurate assays of special nuclear materials (SNM) such as plutonium and uranium. Employing an unwieldy detector on the scene, especially one requiring an external high-voltage power supply or data acquisition system, slows emergency response. The MC-15 portable neutron multiplicity detector, a 2019 R&D 100 Award winner co-developed by Livermore, Los Alamos, and Sandia national laboratories, was designed with threat assessment in mind. The self-contained detector operates from a built-in touchscreen or a networked computer and weighs less than 23 kilograms—the Occupational Safety and Health Administration's single-person lift limit.

MC-15 detects SNM based on the principle of neutron multiplication, where the spontaneous fission in a mass of the material may yield multiple neutrons correlated in time. "Neutrons resulting from a fission chain arrive in bursts that are separated by gaps," explains Livermore physicist Sean Walston, one of the system's inventors. "This pattern of neutron arrival times reveals the characteristics of the material." The MC-15 reports arrival time patterns with a resolution of 100 nanoseconds, providing a smaller, lighter, and faster alternative to competitive multiplicity counters.

Operators can quickly master MC-15's intuitive controls, and the device's power source—hot-swappable, rechargeable batteries—provides 12 hours of energy with continuous operation. "This detector could be used by law enforcement in the United States and worldwide," says Walston. "It would be great for one to be available in most large cities."

Livermore physicist Sean Walston is a co-developer for the MC-15 portable neutron multiplicity detector (shown here measuring a potential nuclear threat in the trunk of a car).

Better Data, Better Detection

The MC-15 detector is named for its 15 neutron detector tubes, which are filled with helium-3 (^{3}He) gas. MC stands for "multiplicity counter" as well as "Mize compromise," to recognize the team member who proposed the final tube arrangement, satisfying each contributor's wish list for optimizing the device. Signals from the detector tubes are tagged with the time and tube number of a detection. These data can be used to estimate chain length and the rate at which the chains occur to quantify the magnitude of danger.

Firmware processes electrical signals from the ^{3}He tubes, updates the data every second, then either stores the data onboard or delivers it over a network, reducing the workload for high throughput with a low power demand. The operating software provides direct access to key calculations in the firmware, yielding qualitative, real-time answers—a distinct improvement over emergency response detectors that require data post-processing.

Data resolution from MC-15 is more precise than from most competitors. In addition, two or more units can be synchronized to double the detection efficiency and significantly improve data quality. Walston explains, “The doubles rate, the detection of two neutrons from the same fission chain, is a measure of data quality in this type of analysis. The probability of detecting one neutron is proportional to MC-15’s detection efficiency. The probability of detecting two neutrons is proportional to the efficiency squared; three neutrons, efficiency cubed; and so on.”

MC-15 advances several steps ahead of competitors by reducing two challenges found in neutron multiplicity data: dead time and double pulsing. Dead time is the reset period during which a ^{3}He tube cannot detect another neutron. Double pulsing occurs when a ^{3}He tube counts two neutrons when only one exists. Therefore, decreasing dead time and double pulsing leads to more precise detection results.

Built for All Environments

To prove MC-15 could perform and provide accurate data in almost any situation, Livermore took the lead in testing the device’s viability in extreme conditions from high heat and humidity to cold, dry, and dusty environments. Vibration tests simulated transportation of the MC-15 by truck, aircraft, and forklift. Researchers even drop-tested the MC-15 detector inside its shipping case onto concrete from a one-meter height. The tests demonstrated MC-15’s successful operation even under harsh conditions.

Although primarily designed for assessing and resolving threats from illegal nuclear development and testing, illicit proliferation of nuclear materials, and attempts at nuclear terrorism, MC-15 is also a valuable research tool. Its ability to reach higher count rates—up to 100,000 per second with minimal dead time—makes the detector suitable for experimental reactors, nuclear waste assessment, radioactive materials screening, and emergency response training.

The device has been used at the Walthousen Reactor Critical Facility at Rensselaer Polytechnic Institute and the National Criticality Experiments Research Center (NCERC) at the Nevada National Security Site (NNSS) to conduct measurements that inform accident prevention plans at nuclear power plants. At NCERC, experiments using MC-15 have also provided important information in support of nuclear threat assessment strategies. Indoor and outdoor field testing at the NNSS Device Assembly Facility has proven MC-15’s ability to measure SNM inside a potential terrorist threat. With additional deployments, the multilaboratory research team expects the portable, easy-to-use MC-15 to be adopted more broadly by the emergency response community.

—Suzanne Storar

MC-15 (black box) is smaller and lighter than competitive neutron multiplicity counters and is designed to be operated in the field for real-time nuclear threat assessment.

Key Words: MC-15 portable neutron multiplicity detector, multiplicity counter, nuclear threat assessment, R&D 100 Award, special nuclear material (SNM), terrorism.

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Expanding Embolization Success

Livermore development team for the IMPEDE® embolization plug: (from left) Thomas Wilson, Ward Small, Jennifer Rodriguez, and Jason Ortega. (Photo by Julie Russell.)

UNCONTROLLED blood flow through vessels damaged by aneurysm leaks, trauma, and other conditions can increase patients' risk of pain, stroke, and death. Embolization, a minimally invasive treatment, alleviates health risks by blocking blood flow in damaged areas so that it can be diverted back through healthy vessels. Established embolization treatments either stimulate clot formation and enable vessel occlusion, or contract the affected vessel, but these approaches may not be completely effective over time. In some cases, blood flow may recur, or patients may suffer significant adverse effects.

Scientists from Livermore and Texas A&M University along with California-based startup Shape Memory Medical, Inc., have improved upon existing technologies with the IMPEDE® embolization plug, winner of a 2019 R&D 100 Award. IMPEDE offers a more advanced occlusion method, allowing physicians to deliver the highest possible material volume to a targeted vessel using a guided catheter smaller than human veins and arteries. In addition to speeding blood clot formation, IMPEDE reduces adverse side effects and better promotes vascular healing. Livermore researcher Thomas Wilson says, "The IMPEDE embolization plug is the culmination of 20 years of biomedical materials research. The lives of many people—possibly tens of thousands—will be made better through this material."

Quick and Effective

The IMPEDE device is composed of an anchor coil, a radiopaque marker band, and a novel polyurethane, shape-memory-polymer (SMP) foam plug capable of expanding up to 100 times its initial volume when in contact with circulating blood. (SMPs are a class of polymeric materials that remember their primary shape after being molded into a second, temporary shape.) During a medical procedure, the embolization plug is placed inside a guided catheter. The physician navigates the catheter through the patient's vessels using x-ray imaging to deliver the plug quickly and accurately to the damaged vein or artery.

Once the target location is reached, the IMPEDE device's helix-shaped anchor coil holds the compressed foam plug in place as the material expands to fill the blood vessel. The foam's high surface area effectively stops blood flow and speeds the body's ability to form a stable clot. The material is also biodegradable, disintegrating slowly into nontoxic compounds until the plug is ultimately replaced with the body's own collagen and connective tissue, and the once-damaged vessel is healed.

Patients typically leave the hospital the day after treatment, as only a small incision in the groin is required to place the device. Available in three sizes, a single IMPEDE plug can treat blood vessels ranging from 2 to 10 millimeters in diameter, while competing technologies may require multiple plugs for the same procedure. The IMPEDE embolization plug was cleared by the U.S. Food and Drug Administration (FDA) in 2018 and has been used successfully on more than 300 patients, with no reported adverse side effects.

Material Mission

The SMP foam used in IMPEDE was developed by Wilson and former Livermore physicist Duncan Maitland—now at Texas A&M University. Funding was provided through grants from the National Institutes of Health and supported by earlier investments from the Laboratory Directed Research and Development Program and the Department of Energy's Office of Science.

Maitland started work on SMP concepts in the 1990s, drawing on expertise in materials for defense applications. In 2000, Maitland was joined by Wilson, who sought to apply his experience in the polymer industry to biomedical materials. "In industry, I made products, such as siding and household items, better through materials research," says Wilson. "At Livermore, I have been able to improve the lives of individual people." Wilson designed the molecular structure that optimized SMP foam performance for embolization use.

Livermore's high-performance computing capabilities played a key role in the research and development effort. Using computational fluid dynamics simulations, the researchers analyzed how treatment with an SMP foam could affect blood flow within a vessel and how well the material supports conditions that promote clotting and occlusion. The computer models included variations in device design, foam densities, and patient conditions to provide clinicians a dynamic view of treatment using SMP foam.

After transferring to Texas A&M University in the late 2000s, Maitland continued SMP experimentation, prototyping, and preclinical studies under an Inter-Institutional Agreement with Livermore. Subsequent improvements to the material included higher biodegradability and hydrophobicity (water resistance). Ultimately, the polymer foam achieved the complete shape recovery needed to expand quickly and completely fill several types of damaged blood vessels. The intellectual property portfolio for SMP foam has grown to more than 70 issued and pending U.S. patents.

Maitland founded Shape Memory Medical (previously called Shape Memory Therapeutics, Inc.) and licensed SMP foam technologies from Livermore to further develop the polymer material as a commercial embolization plug. Wilson credits Maitland for driving the technical success of the device and Ted Ruppel, Shape Memory Medical's chief executive officer, for applying his experience in medical device startups to position IMPEDE in the marketplace.

"IMPEDE would not exist without the invention of SMP foam," says Wilson. "However, the device would not have achieved FDA approval and reached the medical community without Duncan's and Ted's tremendous efforts." During its clinical adoption phase, IMPEDE successfully treated multiple medical cases including a life-threatening dissected aorta and a pulmonary arteriovenous malformation when other devices failed to achieve full blood vessel occlusion. A new device utilizing SMP foam and enabling physicians to embolize longer vessel lengths received FDA clearance in 2019.

—Suzanne Storar

Key Words: aneurysm, blood vessel, embolization, IMPEDE® embolization plug, occlusion, shape-memory polymer (SMP), stroke, R&D 100 Award, Shape Memory Medical, Inc

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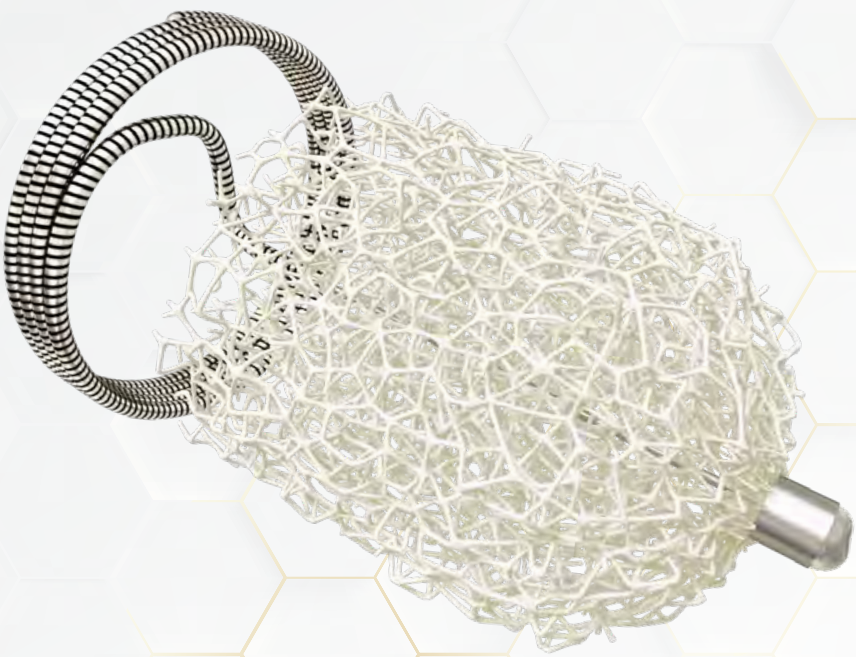
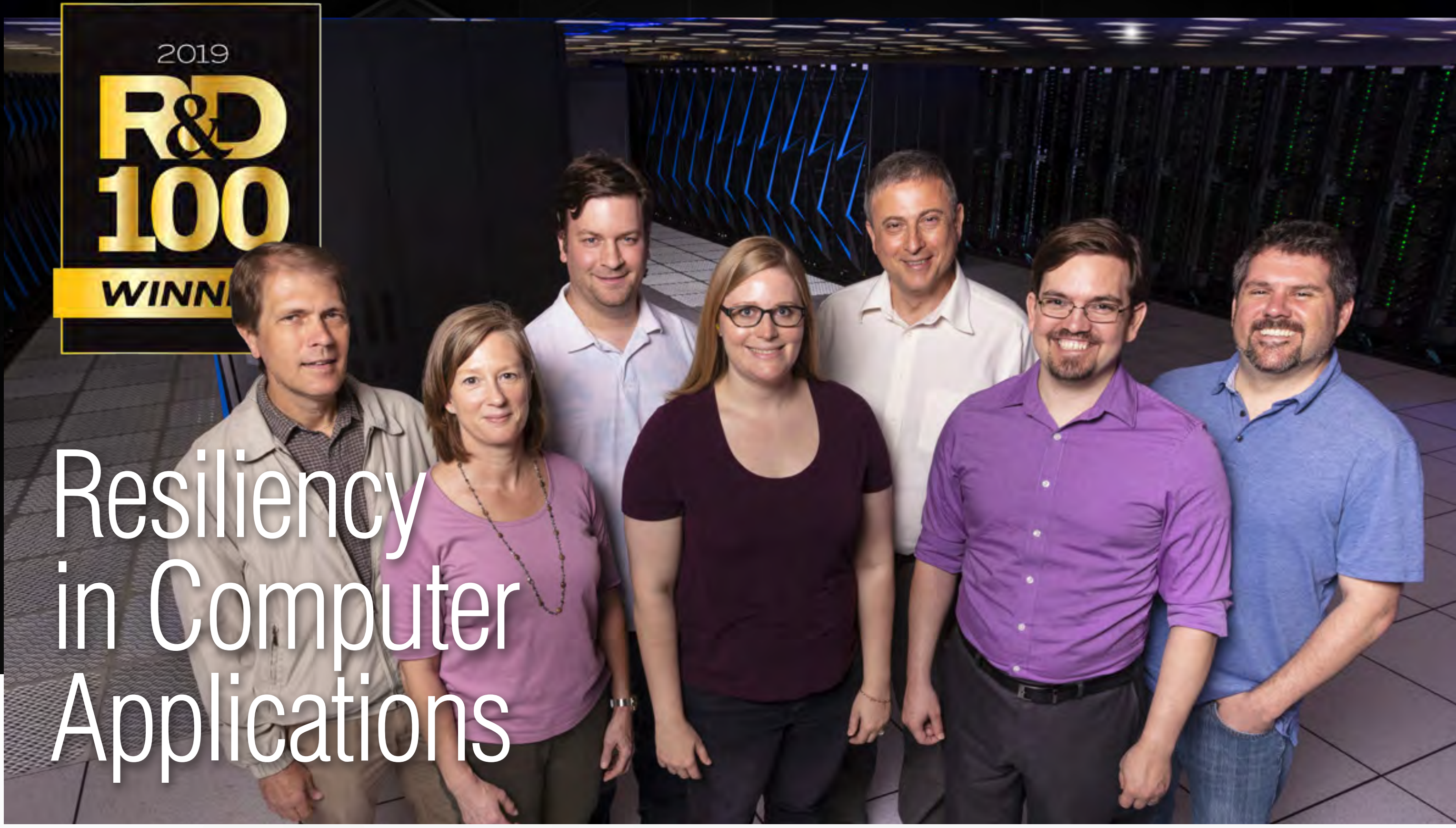
The shape-memory-polymer foam used in the IMPEDE device expands to occlude a damaged vessel, helping the body form a stable clot. The biodegradable plug is ultimately replaced with the body's own



Resiliency in Computer Applications



Development team for Livermore's Scalable Checkpoint/Restart (SCR) framework: (from left) Bronis de Supinski, Kathryn Mohror, Tony Hutter, Elsa Gonsiorowski, Greg Kosinovsky, Cameron Stanavige, and Adam Moody. (Not shown: Greg Becker and Kathleen Shoga.) (Photo by Randy Wong.)

THE stakes are high when scientific applications run on high-performance computing (HPC) systems. Simulations of complex phenomena such as fusion energy and natural disasters require timely analysis to deliver effective solutions. "Checkpointing" techniques help protect against computing failures that slow performance by periodically saving application data as the simulation progresses. When a crash occurs, the application is restarted from the checkpointed file instead of from the beginning—analogous to the way a word-processing program autosaves and subsequently recovers a document.

In traditional checkpointing, application data is saved to and retrieved from the computer's long-term storage—actions known as input/output (I/O) operations. The application waits during this potentially minutes-long process, unable to continue its computations. Researchers must regularly monitor their applications and manually intervene if failures occur to avoid costly slowdowns. "The time to reach a solution matters because scientists need to make time-critical decisions," explains Lawrence Livermore computer scientist Kathryn Mohror, who co-leads the development team behind the R&D 100 Award–winning technology known as the Scalable Checkpoint/Restart (SCR) framework.

Conceived in 2007 by Laboratory computer scientist Adam Moody when a large-scale simulation code failed repeatedly on the Atlas supercomputer, the SCR framework is a multilevel checkpointing system that alleviates the bandwidth bottleneck by caching checkpointed files in storage located close to the compute nodes. The framework leverages short-term storage locations, accelerates I/O operations, and creates failure-resilient checkpoint and restart support. Mohror, who has co-led the project with Livermore computer scientist Elsa Gonsiorowski since Moody stepped down from the position in 2019, says, "Simulations can be completed more quickly with a smarter checkpointing system like SCR."

Full Feature Set

On a supercomputer, checkpointed files are saved in a complex, hierarchical storage architecture. SCR manages the movement of checkpointed files through the storage hierarchy to achieve the best performance for the application. This process involves executing many complex tasks while the application runs—performing health checks of the computing environment, monitoring the application's progress, managing I/O data, and transferring data—and exploits storage levels that are not shared across all of a supercomputer's nodes. In addition, SCR saves only the checkpointed data needed at the time, not the entire system state. "In most cases, SCR can restore a checkpoint from short-term storage because most failures affect only a small part of the application at a time," notes Mohror. SCR can also fall back to checkpoints in long-term storage, if necessary.

SCR is further differentiated from other checkpointing tools by its I/O management techniques, including the types of output files it handles. Mohror explains, "With our latest software release, SCR manages more than checkpointed files to storage. Now, it also manages general files containing other simulation data." SCR's I/O mechanisms scale linearly with the number of compute nodes used by the application and are as much as 1,000 times faster than I/O operations that do not use SCR. This enhancement allows researchers to output higher resolution data more frequently from their application runs, leading to a better understanding of the results.

Moreover, SCR accommodates different types of HPC storage architectures and their resource management configurations. Mohror says, "For each storage device, system administrators can specify the device's size, its failure characteristics, and how many checkpoints to store before deletion." SCR's checkpointing mechanisms "wrap" around the code, independent of the device or operating system. No two supercomputers are alike, and such software portability techniques are crucial for adapting Livermore's codes to future exascale-class machines.

From the user's perspective, SCR offers a flexible application programming interface that easily integrates into an application's existing I/O code. The user specifies a few parameters that tell the computer when, where, and how often to capture checkpoints. No other code modifications are needed. Ultimately, the user does not need to understand or manage the computer's specific storage hierarchy and can instead focus on the scientific application.

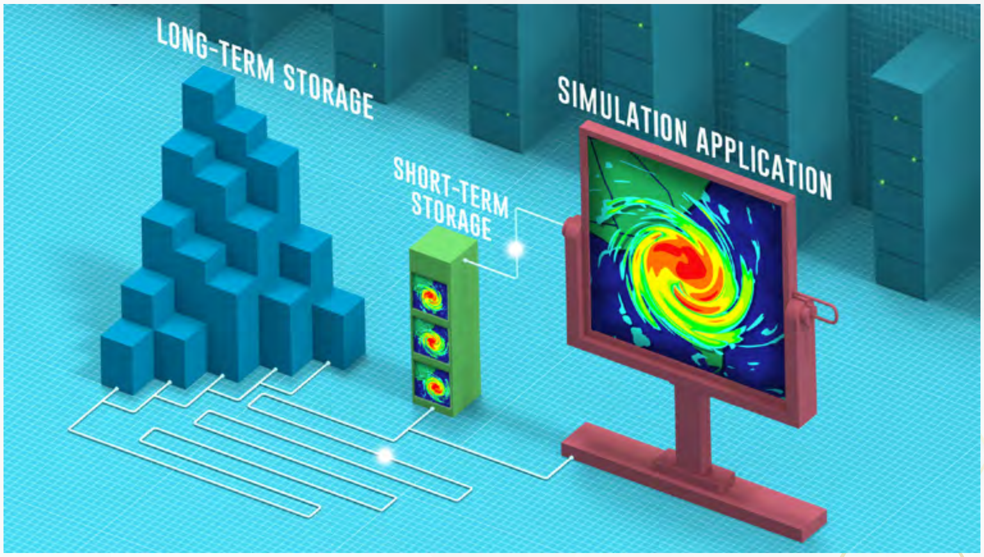
Proof in Production Codes

Livermore's pF3D code, used by the National Ignition Facility to simulate backscatter from laser light, was the first production code to use SCR. When a new supercomputer came online in 2007, Moody explains, "Each pF3D calculation needed days to complete, but the system failed every few hours. SCR saved and protected each checkpoint against system failures using data redundancy encodings." SCR reduced pF3D's checkpoint and restart time from more than 10 minutes to just seconds, allowing checkpointed files to be saved more frequently. Livermore physicist Denise Hinkel recalls, "I had been setting alarms to check the pF3D simulation periodically throughout the night, like it was a newborn baby. SCR's automated checkpoints and restarts let me sleep again."

SCR provides faster checkpointing, faster restarts, and portability across computing platforms. "We see orders of magnitude improvement in performance when using SCR, especially when running extremely large-scale applications," states Mohror. Such improvement is especially important as existing codes are modified for next-generation machines. For example, SCR sped up pF3D's checkpointing time by 48 times on Atlas and 19 times on an HPC system called Hera.

After more than a decade supporting a variety of applications and computing systems, SCR continues to evolve. Mohror states, "We want SCR's data management infrastructure to support even more complex workflows." As open-source software, the framework's influence can extend beyond the Laboratory. (See *S&TR*, January/February 2018, pp. 4–11.) Located at the University of California at San Diego, the San Diego Supercomputer Center is an example of an academic partner using SCR on production HPC applications. The application is useful for industry as well. Moody notes, "Our solution has worked so well that we want more people to benefit from it."

—Holly Auten



SCR leverages short-term storage for checkpoint files, thus accelerating data retrieval and subsequent restarting of the application if a computing failure occurs. The white dots represent data input/output movement between storage tiers and the scientific application. (Rendering by Ryan Goldsberry.)

Key Words: application programming interface, Argonne National Laboratory, checkpointing, high-performance computing (HPC), input/output (I/O) operation, open-source software, pF3D code, R&D 100 Award, Scalable Checkpoint/Restart (SCR) framework, scientific application, simulation.

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Software Installation Simplified

Development team for Spack: (from left) Greg Lee, Matt Legendre, Todd Gamblin, Peter Scheibel, Greg Becker, and Tamara Dahlgren. (Photo by James Chalabi.)

HIGH-PERFORMANCE computing (HPC) centers, such as Lawrence Livermore's, routinely deploy large-scale scientific software applications. These applications rely on tens to hundreds of external programs, known as packages, that enable the computer's operating system to execute specific functions and perform as needed. Packages include software versions tailored specifically for users' machines as well as dependencies and configurations customized for their applications. Even for seasoned professionals, manually downloading, installing, building, and resolving conflicts among all of these programs is onerous, and this time-consuming process is a substantial barrier to scientists.

Spack, a 2019 R&D 100 Award–winning software technology, was created to alleviate the package managment burden. "The inefficiency and complexity of building software for HPC machines can detract from scientific research," explains Livermore computer scientist and Spack principal investigator Todd Gamblin. "Spack's automated package management eliminates much of the grunt work."

Codeveloped by a dozen other universities, national laboratories, institutes, and computing centers, Spack also won a silver medal in the R&D 100 Awards' Market Disruptor category.

Gamblin notes that other package managers can only be run by administrators and other privileged users and do not handle simultaneous custom installations of multiple software versions and configurations. Fortunately, Spack is designed for these scenarios and can be used by nonprogrammers, developers, and system administrators alike. Users need only download the Spack tool and learn its specification syntax.

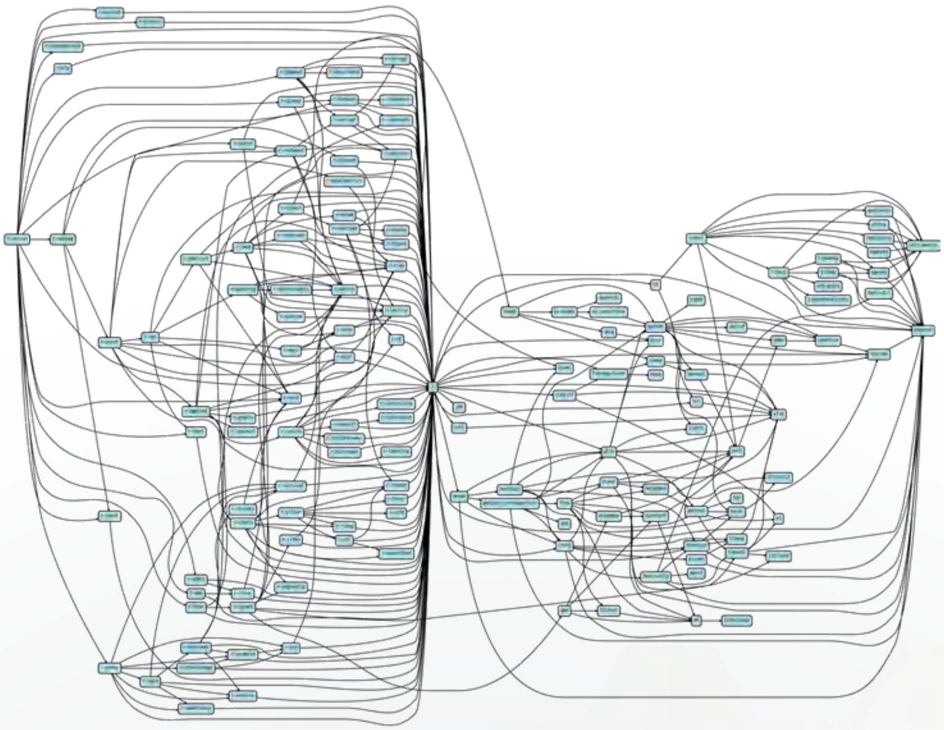
Complexity Behind the Scenes

Installing and using software dependencies is a careful balancing act as new packages are integrated into an application and each addition increases the complexity of the task. Spack speeds up installation by assembling all the packages needed for an application's deployment, managing their configurations, and optimizing the build for the user's machine. The user views and queries Spack's list of available packages, then Spack automatically downloads and builds source code for the desired packages' dependencies. Users can assemble hundreds of software libraries in minutes, giving them more time to focus on their scientific research.

Spack's recipes—steps for building a package—are written in the widely used Python programming language. On top of Python, Spack provides its own domain-specific language that enables contributors to write templated instructions, so a single recipe file can be used to build many different configurations. (Other package managers can require thousands of duplicate files to accomplish the same task.) To build a configuration, Spack offers a custom specification language for selecting options, versions, and compilers. Gamblin states, "Together, Spack's package recipes and specification syntax allow users to tailor their software stack for specific codes and computing environments."

Spack's concretization algorithm is responsible for converting the user's abstract requirements into concrete, buildable specifications. The process effectively fills in the blanks of software configuration. The user provides a partially completed form, and the algorithm finds a configuration that satisfies the user's requirements as well as each package's unique compatibility rules. The algorithm produces an output file of the resulting configuration data, allowing users to easily reproduce a software stack for a particular scenario.

Perhaps Spack's most impressive feature is its repository of thousands of templated packages supporting diverse computing platforms (including laptops), simulation frameworks, programming languages, and other options. Gamblin explains, "A user's software integration burden increases with every new library or update, but Spack manages the growing complexity and allows users to build quickly on a variety of computing systems."



A typical multiphysics code used at Lawrence Livermore requires installation of hundreds of software packages and dependencies, as illustrated by this map of the "rminer" package. Whereas manual installation of such complex software would be impossible, Spack's automation makes quick work of the task.

Worldwide Impact

Spack's features and flexibility have led to its adoption by many prominent coding teams, supercomputing centers, and software development communities at Livermore and beyond. For example, Oak Ridge National Laboratory uses Spack to deploy more than 1,300 software packages on the top-ranked Summit supercomputer. This installation process previously required two weeks of work and can now be deployed overnight. Spack is also used at Los Alamos National Laboratory, Fermi National Accelerator Laboratory, CERN (the European Organization for Nuclear Research), and the Japanese research center RIKEN.

The Spack team regularly offers tutorials and workshops at major supercomputing conferences and visits HPC centers to learn from and train development teams. Spack is used for software deployment on 6 of the world's top 10 supercomputers and has been adopted as the standard deployment tool of the Exascale Computing Project (ECP)—a Department of Energy collaboration tasked with building a reliable software stack for future exascale-class machines. According to ECP deputy director Lori Diachin, "Spack is an integral part of the ECP's ecosystem because our software stack is quite large and complex."

Spack is open-source software, which means its functionality can expand and its features can mature thanks, in part, to the software community beyond the Laboratory. (See also the article on p. 8 of this issue; *S&TR*, January/February 2018, pp. 4–11.) Spack has more than 500 contributors and 2,000 monthly active users around the globe—and the numbers are growing."Learning about use cases at research institutions and other HPC centers has helped us make Spack what it is today," says Gamblin. "Open-source development benefits those who use and contribute to Spack."

Next-generation HPC architectures, with diverse graphics processing units and accelerators, will only increase the complexity of scientific applications and the necessary software dependencies. As the bar is raised, Gamblin expects Spack to become smarter and more automated. He states, "We are always expanding Spack's capabilities to adapt to new technologies and user needs."

—Holly Auten

Key Words: compiler, concretization algorithm, Exascale Computing Project (ECP), high-performance computing (HPC), open-source software, package, package manager, R&D 100 Award, software installation, software stack, Spack.

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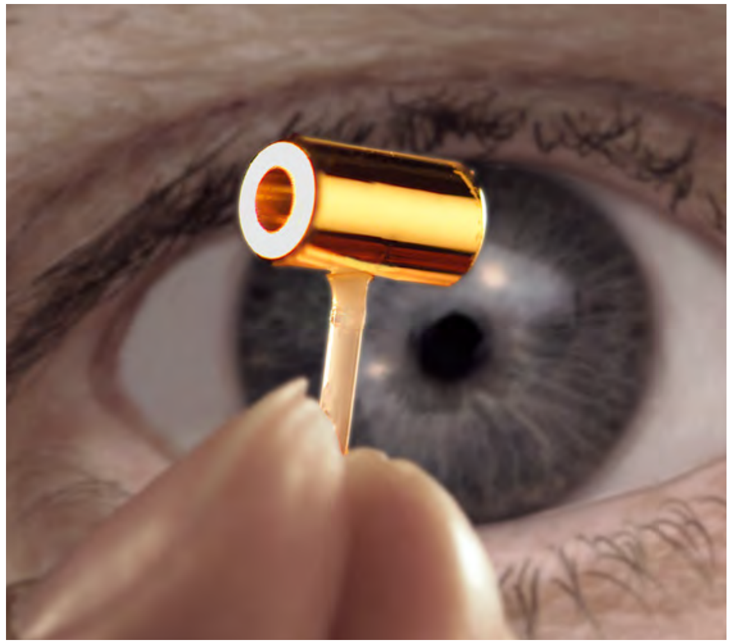
The Shape of

RE-CREATING a miniature version of the Sun's nuclear-fusion power source in a laboratory setting has been a long-standing scientific goal. At Lawrence Livermore's National Ignition Facility (NIF), scientists have made exciting progress toward achieving ignition—a self-sustaining nuclear-fusion reaction—through inertial confinement fusion (ICF) experiments.

In indirect-drive ICF experiments, NIF's 192 high-power laser beams are used to heat and compress a deuterium–tritium (DT) fuel capsule seated inside a cylindrically shaped device called a hohlraum. The beams enter through holes on either end of the hohlraum, strike the cylinder's inner walls, and generate a bath of x rays. The x rays converge symmetrically on the capsule, which implodes, heating and compressing the DT fuel into a central hot spot, wherein fusion begins.

Over the years, innovative and pioneering NIF researchers have continued to advance the ICF effort, seeking improvements in all aspects of the experiments, from target design to data acquisition and analysis. Now, scientists are turning their attention to how changes to

Things to Come



A typical hohlraum cylinder is just a few millimeters wide with laser entrance holes at either end. The deuterium–tritium fuel capsule (not shown) is seated inside the hohlraum for inertial confinement fusion (ICF) experiments at the National Ignition Facility (NIF).

the hohlraum could further improve target performance, sparking new optimism in efforts to create a star on Earth—an achievement that could open the door to nearly limitless energy production.

Focusing on Ignition

During ICF experiments, fusion reactions within the hot spot produce alpha particles (helium nuclei) and neutrons. The number of neutrons generated characterizes the extent of the fusion process. For ignition, enough alpha particles must be present to initiate further fusion reactions in the hot spot and create a thermal runaway effect. Recent NIF experiments have reached the "alpha-heating regime," in which the self-heating by fusion products dominates near the center of the fuel, with neutron yields exceeding 1×10^{16}. However, yields must be higher for ignition, and the target capsule's inefficient absorption of the x rays is a limiting factor.

Of NIF's initial 2 megajoules of laser energy, about 1.6 megajoules are converted to x rays in the hohlraum. The capsule then absorbs only about 150 kilojoules, which is approximately 10 percent of the laser energy provided by NIF. "We lose a lot of energy in the coupling of the hohlraum x rays to the capsule," notes Livermore physicist and hohlraum designer Peter Amendt. Increasing the energy efficiency of this coupling would benefit the central hot spot approach, in which an ignition spark initiates propagating thermonuclear burn. The energy boost would also support research on using a double-shell capsule to volumetrically ignite the whole fuel at once.

Shape Changers

One way to improve coupling efficiency of the x rays to the capsule is to increase the capsule size. However, the capsule's diameter, typically 2 millimeters, is constrained by the hohlraum's usually cylindrical shape. Simply increasing the capsule's diameter leads to an uneven distribution of x rays around it, resulting in an asymmetrical implosion that degrades the fusion process and inhibits ignition.

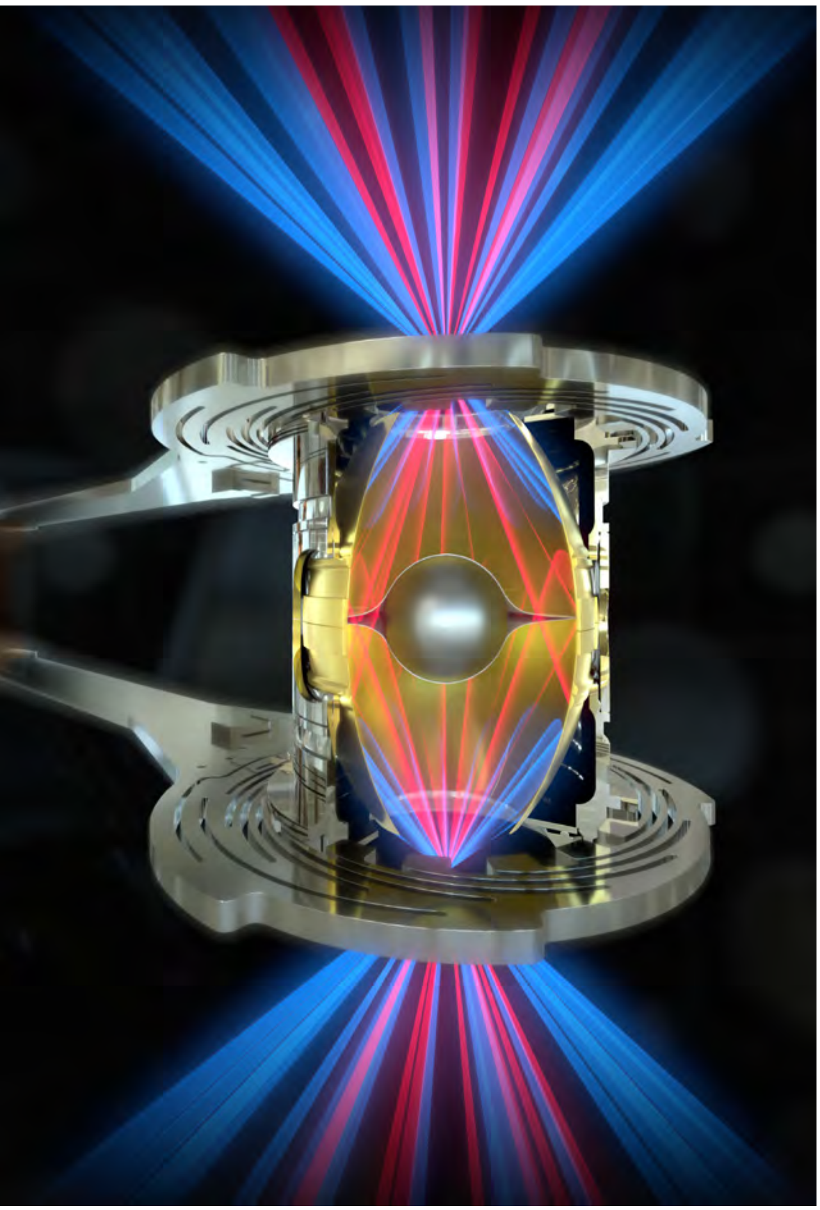
To increase the capsule's size and ultimately the amount of laser energy absorbed, scientists, including Amendt, had to take an "out-of-the-box" look at the shape of the hohlraum. Four years ago, in a study funded by the Laboratory Directed Research and Development (LDRD) Program, Livermore's Ogden Jones considered several novel hohlraum designs, including a nested spherical hohlraum or "ballraum" and a "midraum" cylinder bristling with periscope-like entry tubes for the shallow-angle laser beams. A more recent LDRD project headed by Amendt focused on two next-generation hohlraums that appeared to provide high-coupling efficiency—the rugby ball–shaped hohlraum, which is wider at the center and tapered toward both ends, and the frustraum, which looks like two identical truncated cones joined at their largest diameter.

The rugby hohlraums were implemented in studies to better understand how the outer shell of a future double-shell ignition target would behave. For these experiments, Livermore physicists Yuan Ping and Vladimir Smalyuk used a 7-millimeter-wide gold rugby hohlraum with a fuel capsule 3.5 millimeters in diameter—50 percent larger than a traditional capsule. This larger capsule held more fuel and had a greater surface area for capturing x-ray energy. The laser pulse shape used to drive the target was also slightly different. With cylindrical hohlraums, pulse shapes typically start with a few small power peaks followed by a main peak at about 10 nanoseconds to gently form and maintain a dense DT fuel layer. For the rugby hohlraum experiments, a short, high-power pulse was delivered to the capsule earlier in the implosion process, resulting in better coupling.

The 1-megajoule laser shots resulted in 300 kilojoules being absorbed by the capsule—increasing the energy coupling to 30 percent. "We set a new energy coupling record for a hohlraum," says Amendt. The team plans to step up the total amount of laser energy while determining the right combination of laser pulse shape, capsule size, and rugby hohlraum shape to achieve a symmetric implosion. Collaborating closely with Los Alamos National Laboratory scientists, the team is optimizing the energy delivery to the capsule to enable volumetrically igniting the fuel. In addition, with more energy available, defects can be better tolerated, providing more margin of error to achieve ignition.

Amendt also directs the design effort for the frustraum, a close cousin of the rugby hohlraum, with Livermore's Steve Ross leading the experiments and Darwin Ho optimizing the capsule design. Amendt explains that the frustraum's unusual shape has several benefits. The large central volume allows an oversize capsule to be easily fielded, promoting more x-ray absorption. The frustraum also uses smaller laser entrance holes, which reduces the ability for x rays to escape.

Another key feature is that the frustraum could generate more "specular glint" than cylindrical hohlraums. Specular glint is unabsorbed laser light that hits and reflects off the hohlraum's inner walls at the same angle it entered the hohlraum. According to



An artist's rendering shows NIF's 192 laser beams entering a gold-lined rugby hohlraum holding an aluminum fuel capsule. (Red and blue lines represent the inner and outer beams, respectively.) These hohlraums are wide at the center and tapered toward the ends. This shape is one of several under development for improving the energy efficiency and symmetry of ICF implosions. (Rendering by Jacob Long.)

simulations, this reflected light might help with symmetry by conditioning the hohlraum plasma, allowing better propagation of laser light to the frustraum waist. Simulations calibrated to the earlier rugby-shaped hohlraum experiments suggest that the frustraum could offer effective symmetry control and sufficient drive to provide high-yield, moderate convergence implosions. For comparison, the standard convergence in a cylinder would be like squashing a basketball to the size of a pea. "With the frustraum, we may need only to shrink that basketball down to the size of a marble to achieve the same result," explains Amendt.

Two 1.5-megajoule shots at NIF in early 2019 with 7-millimeter-diameter frustraums provided encouraging data for this design, yielding nearly 500 kilojoules of energy on target—far higher than any on-target results in the past. "We're aiming for more efficient hohlraums," said Amendt. "A more efficient hohlraum gives us a higher performance margin. Too little margin doesn't give us enough leeway to handle all the aspects that can interfere with getting the maximum efficiency, such as pre-heating the fuel. With a bigger capsule, we can tolerate more pre-heat on the path to ignition."

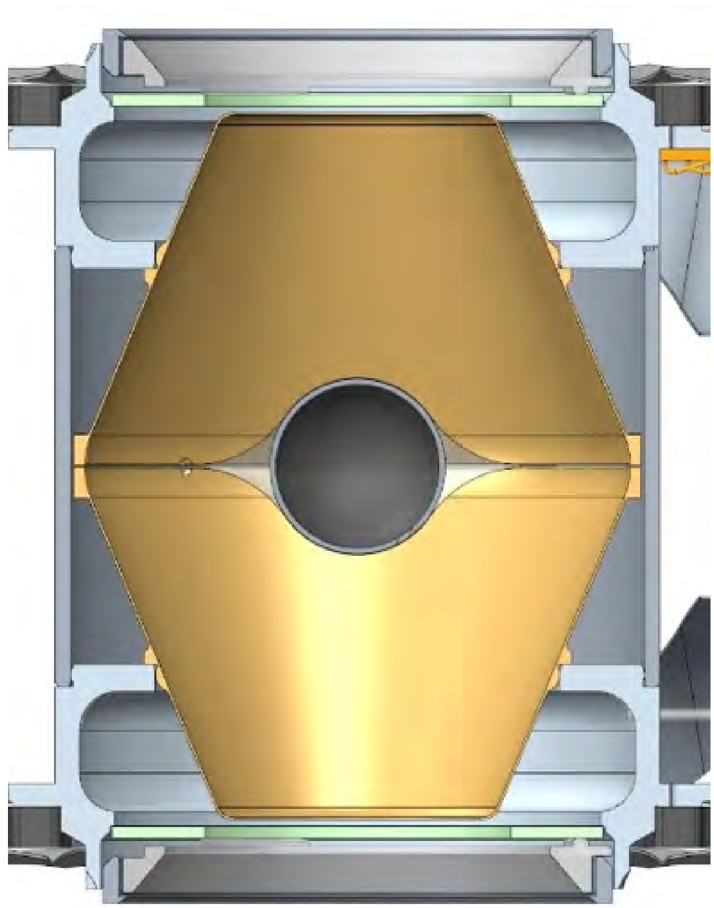
Future Looks Bright

With the rugby hohlraum showing promise as an option for use with double-shell targets and the frustraum offering more efficiency for hot spot ignition, research on these new designs continues in earnest at NIF. Three subscale frustraum shots were completed in May 2019. During these experiments, the team met its three primary goals: achieving acceptable levels of backscattered laser light; demonstrating nearly 20 percent coupling efficiency; and developing a "peg" point for the simulation codes to predict, with improved confidence, symmetric drive conditions at full scale.

With these challenges met, a full-scale frustraum campaign is under way for the ICF Program. During this campaign, a 9.3-millimeter-diameter frustraum will be fielded with a 2.6-millimeter capsule to further refine modeling tools. Testing will address the accuracy of the models regarding key physics issues such as implosion symmetry, while planned experiments using the OMEGA laser at the University of Rochester's Laboratory for Laser Energetics will focus on improving the basic physics understanding of specular glint in frustraums. Experiments using 3-millimeter-wide capsules in a rugby hohlraum are scheduled at NIF in 2020 to explore volume ignition in single-shell targets.

Amendt notes that these new ideas and approaches had their birth in LDRD projects. "LDRD gives us the opportunity to engage in 'disruptive research,' and to propose unusual ways to solve complex challenges," he explains. "Now, we are looking at tripling the absorbed energy and tripling the performance margins. This increased performance margin will give us room to accommodate tiny target imperfections and our imperfect knowledge of the microphysics involved." With a 300-percent leap in both energy absorption and performance margin, Amendt adds that the 2-megajoule NIF facility can provide capabilities that had previously required 6 megajoules, at no extra cost. He states, "The benefits are so great, we are determined to give this effort our best shot."

—Ann Parker



The frustraum design could reduce the amount of energy absorbed by the hohlraum's inner walls, improve the implosion symmetry of the fuel capsule (grey circle), and reduce the amount of backscattered laser light compared to traditional cylindrical hohlraums.

Key Words: frustraum, hohlraum, inertial confinement fusion (ICF), National Ignition Facility (NIF), OMEGA laser, rugby hohlraum, specular glint.

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Tuning into Dark Matter

IN the 1930s, Swiss astrophysicist Fritz Zwicky posited that an invisible substance was responsible for the unobservable mass in galaxy clusters that kept them from breaking apart. Deemed "dark matter," this substance consists of mysterious particles that emit no light and have an unspecified form, providing scientists with the monumental challenge of proving it exists. Even now, decades after Zwicky's discovery, astrophysicists have yet to directly observe dark matter or determine its composition.

To help solve the mystery, Lawrence Livermore researchers, in collaboration with colleagues at the University of Washington, Fermilab, Los Alamos and Pacific Northwest national laboratories, the University of Florida, Washington University in St. Louis, the University of California (UC) at Berkeley, and a few international institutions, are searching for the axion—a low-mass particle that could make up the majority of dark matter. Funded by the Department of Energy's Office of Science, the team has developed a novel particle detector, called the Axion Dark Matter Experiment (ADMX), to identify axions' decay into microwave-frequency photons in the presence of a strong magnetic field, thus providing a measurable signature. (See *S&TR*, January/February 2015, pp. 23–26.)

A Whisper in a Rock Concert

Scientists hypothesized the plausible existence of the axion while trying to solve a different particle physics problem. A neutron, which is a composite particle of three quarks with positive and negative charge, should exhibit some charge separation that presents as an easily measured dipole moment. Instead, the scientists measured no dipole moment. Follow-on experiments indicated that the maximum dipole moment would be at least 10 orders of magnitude smaller than expected, leading scientists to theorize that the field of a hypothetical particle, dubbed the axion, was affecting that value. The axion's predicted characteristics—ability to couple with photons, rare interactions with regular matter, and extremely light mass—coincidentally matched those of potential dark matter.

If axion particles decay into photons as scientists expect, the interaction would produce a tiny but detectable signal in the form of a microwave. In nature, this process would be nearly impossible to detect—the half-life of an axion would be greater than 10^{50} years. However, in 1983, theorist Pierre Sikivie of the University of Florida suggested an experimental method to boost the axion's signal. The proposed axion "haloscope" uses an extremely strong

The Axion Dark Matter Experiment (ADMX) uses a haloscope that consists of a large-diameter solenoid magnet with a copper-plated, frequency-tunable microwave cavity at the center. Pictured with the device are team members (from left) Nathan Woollett, Jenny Smith, Rakshya Khatiwada, and Sophia Schwalbe. (Photo by George Kitrinos.)

magnet, essentially a dense field of photons, to stimulate the axion decay to detectable levels.

Several proof-of-concept haloscopes were built to demonstrate the technique, and the official ADMX detector was built at Lawrence Livermore in the early 1990s. ADMX consists of a large-diameter solenoid magnet with a copper-plated, frequency-tunable microwave cavity at the center. "Our technology is effectively an ultrasensitive AM radio," says Gianpaolo Carosi, a Livermore staff physicist and co-spokesperson for the ADMX effort. "The axion signal is similar to an extremely weak radio wave. It's so faint that it doesn't couple to ordinary antennas, so we have to amplify the signal to hear it."

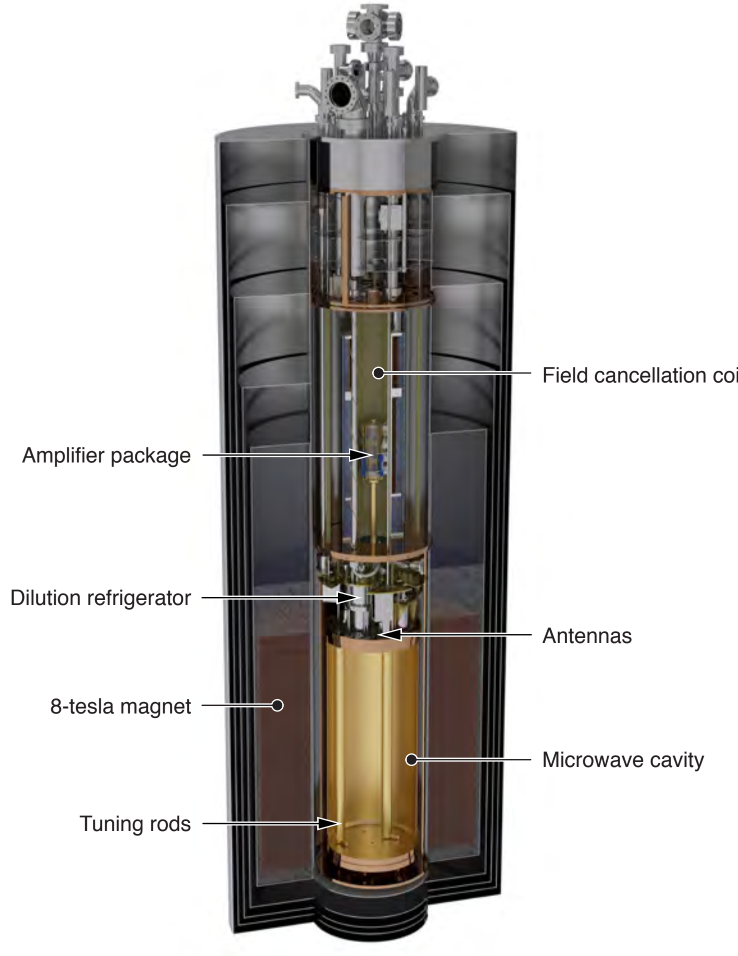
ADMX uses an 8-tesla magnet to stimulate the decay of axions into photons. (For comparison, the Earth's magnetic field is only 10 to 65 microteslas.) The microwave cavity contains two tuning rods. Scientists move the rods on axles from the edge of the cavity to its center so they can "tune in" to the relevant frequencies in which they believe axions exist. To ensure the fidelity of the detector, scientists periodically inject radio signals with the same expected power as the axion. The haloscope's automatic algorithm detects the synthetic signals, which helps to calibrate the system and verify its functionality.

Enhanced Detection Capabilities

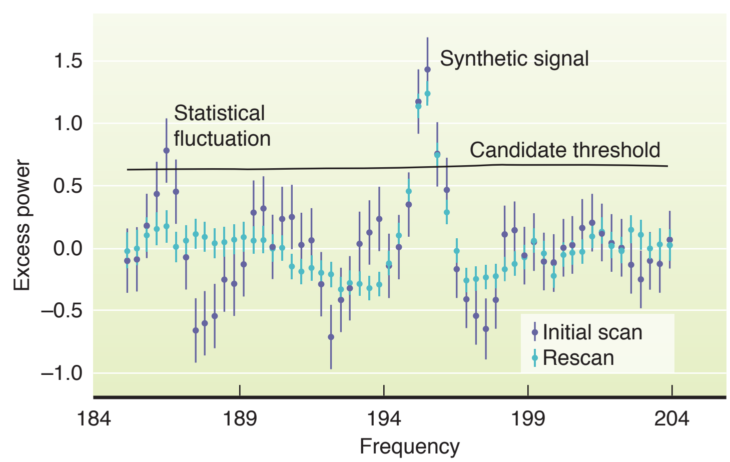
Scientists have made an educated guess about the frequency range of axions using various clues provided by astrophysics. "Observations of motion in the galaxy allow us to approximate the amount of dark matter that exists and how it is moving around in the universe. Since axions are bound in the galaxy, the width of the signal (through added kinetic energy) can't be broader than 1 or 2 kilohertz for an axion that converts to a 1-gigahertz photon," says Carosi. "The frequency range is based on the assumption that the axion forms the majority of dark matter. If we don't detect the axion, then the particle is not likely the primary source."

Recent technological advances have helped the research team reach a point where finding the axion is just a matter of time. "Part of the challenge, and the reason why this experiment has taken decades to accomplish, is the instruments we use produce heat and background noise that can cover up the signal we're trying to measure," says Carosi. Counteracting thermal interference from the cavities is straightforward—scientists incorporated dilutional refrigerators into the system that cool it to around 100 millikelvins—but mitigating the background noise produced by the amplifiers proved a bigger challenge.

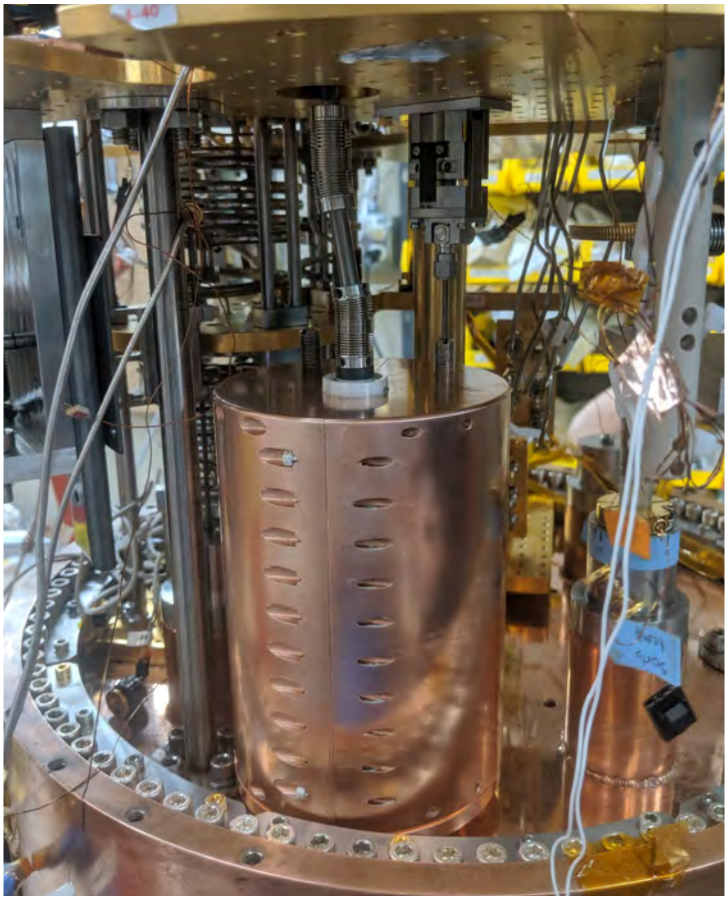
UC Berkeley professor John Clarke revolutionized the search for axions when he developed a microstrip superconducting quantum interference device (SQUID) amplifier that drastically reduced the thermal noise in the cavity.



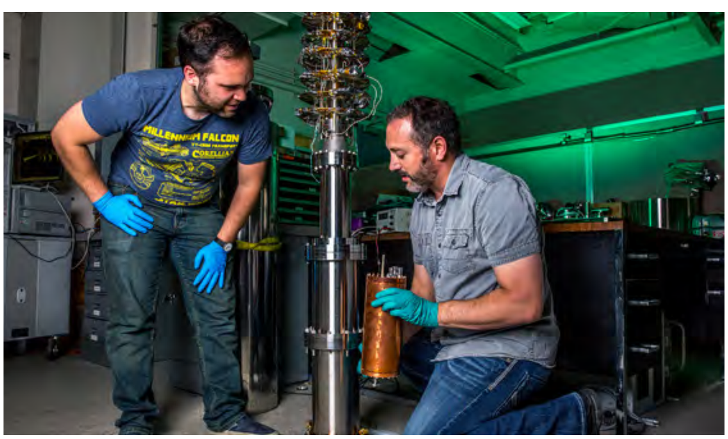
A rendering of the ADMX detector's interior highlights its many components, which are stacked into a several-meters-long instrument. (Image courtesy of the ADMX collaboration.)



An initial scan of ADMX data (purple markers) showed two frequency regions with excess power above a set threshold, indicating potential axion candidates. A subsequent rescan (blue markers) clarified that one candidate was a statistical fluctuation, while the second candidate was the result of a purposefully injected tone acting as a synthetic axion signal.



The ADMX sidecar cavity allows scientists to test improvements to the ADMX system in situ without affecting the main experiment.



Livermore scientists Woollett and Gianpaolo Carosi work on the cryostat system in which the test microwave cavity (copper cylinder) will be placed. (Photo by George Kitrinos.)

(See *S&TR,* December 2018, pp. 4–11.) Previous transistor-based amplifiers only reduced the thermal noise to temperatures around 2 kelvins, but quantum amplifiers can reduce it close to the quantum limit—around 50 millikelvins at 1-gigahertz frequency. The current ADMX system uses both SQUID and Josephson parametric amplifiers to boost the signal to detectable levels. These modifications have enhanced the system's effectiveness so that if axions are found, their signature will be unmistakable.

Listen and Learn

The team is now scanning the first frequency range (between 0.6 and 2 gigahertz), eagerly anticipating the detection of an axion. While they collect and analyze the incoming data, the researchers continue to make additional system improvements using a "sidecar" testbed cavity—an endeavor led by Livermore scientist Nathan Woollett. The sidecar is installed right above the main ADMX cavity, which allows scientists to test new technologies within the main ADMX system without affecting the experiment. Sidecar testing has resulted in multiple advances, including a piezoelectric actuator for moving the tuning rods that is simpler and more compact than its predecessor. The team is also testing a two-cavity design that would boost the detectable frequency range for the next ADMX data run, as well as other improvements such as modifying the shape of the cavity itself to enhance its resonance.

Since the sidecar is connected to ADMX and runs simultaneously, it has the potential to discover new particles in a different frequency range than the main system. "The sidecar cavity is unique—although it's not sensitive to the standard axion, it is sensitive to axion-like particles, which could provide a brand-new particle result," says Woollett.

ADMX will test millions of frequencies across multiple data runs in the coming years. If the axion is detected, this team would be the first to prove the existence of dark matter—a groundbreaking achievement—and set the stage for seemingly boundless investigations into the axion's properties. Such an achievement would also open the door to new exploration. Carosi says, "We could learn how the galaxy is made, see which direction dark matter is going, and maybe even find useful applications for navigation…the possibilities are tremendous."

—Lauren Casonhua

Key Words: axion, Axion Dark Matter Experiment (ADMX), dark matter, haloscope, microwave cavity, quantum amplifier, superconducting quantum interference device (SQUID).

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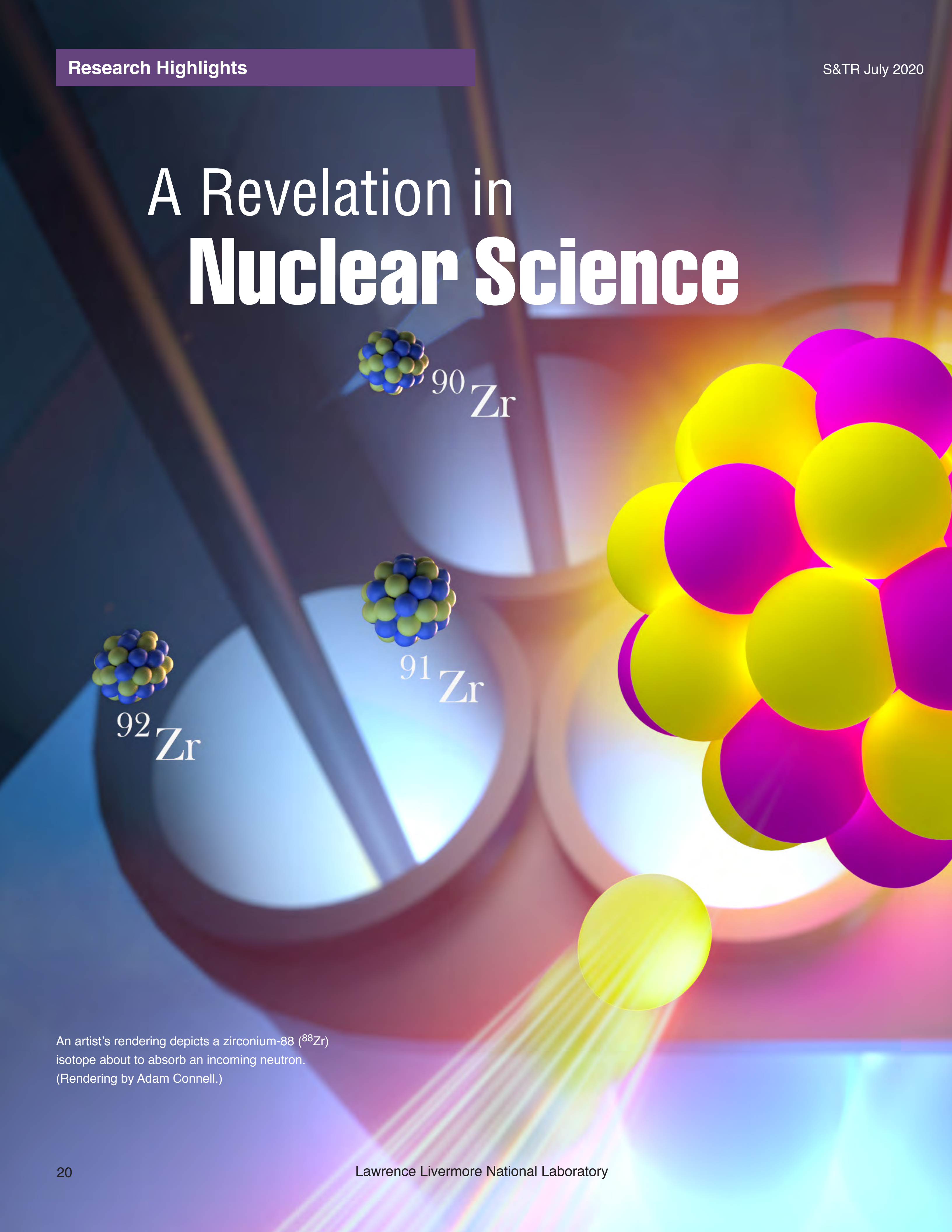
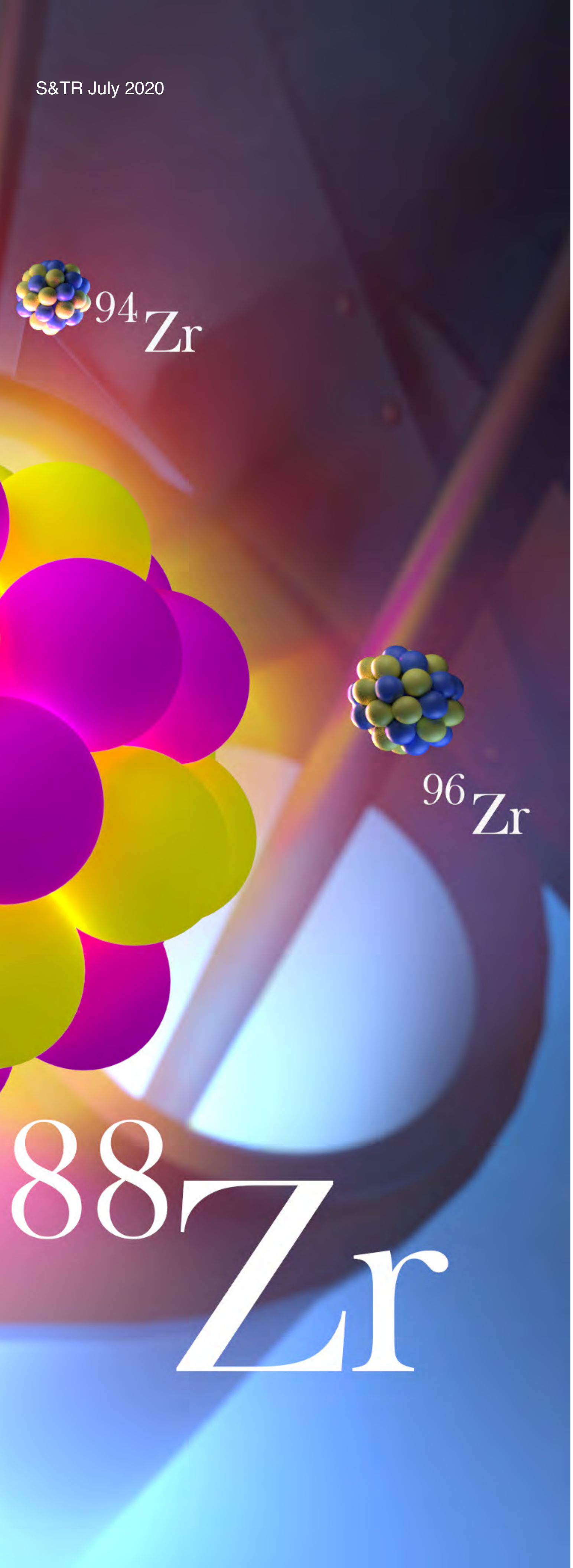
A Revelation in Nuclear Science



An artist's rendering depicts a zirconium-88 (^{88}Zr) isotope about to absorb an incoming neutron. (Rendering by Adam Connell.)



WHEN it comes online in 2022, the Facility for Rare Isotope Beams (FRIB) at Michigan State University (MSU) will give scientists an unprecedented capability to produce and "harvest" rare, or exotic, isotopes—highly unstable nuclei that are not typically found on Earth. Such investigations are essential to better understand fundamental nuclear science and could give rise to new applications in areas ranging from astrophysics to national security.

In anticipation of FRIB, scientists are conducting preliminary experiments at established accelerator facilities, including MSU's National Superconducting Cyclotron Laboratory (NSCL). At this facility, beams of heavy ions are accelerated toward and collide with a target material. The collisions cause the nuclei in the ions to break apart, shedding neutrons and protons, and the resulting nuclear fragments yield different types of radioactive isotopes. Many nuclear scientists are interested in searching for the limits of nuclear stability by studying isotopes with the greatest neutron-to-proton imbalance, but researchers are also looking into how to collect the copious other products for basic and applied science research. "For each extremely exotic nucleus that is created, vast quantities of long-lived radioactive nuclei are also produced," says Livermore nuclear physicist Nicholas Scielzo.

In an experiment conducted at NSCL in 2018, Livermore researchers, in collaboration with several university partners, successfully used a water-based harvesting apparatus to collect zirconium-88 (^{88}Zr) atoms, which under normal operations would have been "filtered out" from the more exotic products. Scielzo, who leads the Livermore research team, says, "We are developing

Livermore scientists, in collaboration with university partners are studying ways to harvest rare isotopes, including a radioactive isotope of the element zirconium.

the techniques needed to harvest isotopes such as zirconium-88 that are closer to stability, and we are demonstrating that these harvested samples can then be used for direct neutron-capture measurements."

An isotope's neutron-capture cross section—the likelihood that a nucleus will absorb a neutron—is important to many scientific processes, such as the forging of elements in the cosmos, and to applications of nuclear science spanning reactor performance, nuclear medicine, and stockpile stewardship. Although cross sections have been established for most stable nuclei, almost no data exists for radioactive isotopes, including ^{88}Zr, which serves as an important radiochemical diagnostic for nuclear security applications. In pursuing this data, nature handed the research team an incredible surprise: the second largest neutron capture rate ever measured.

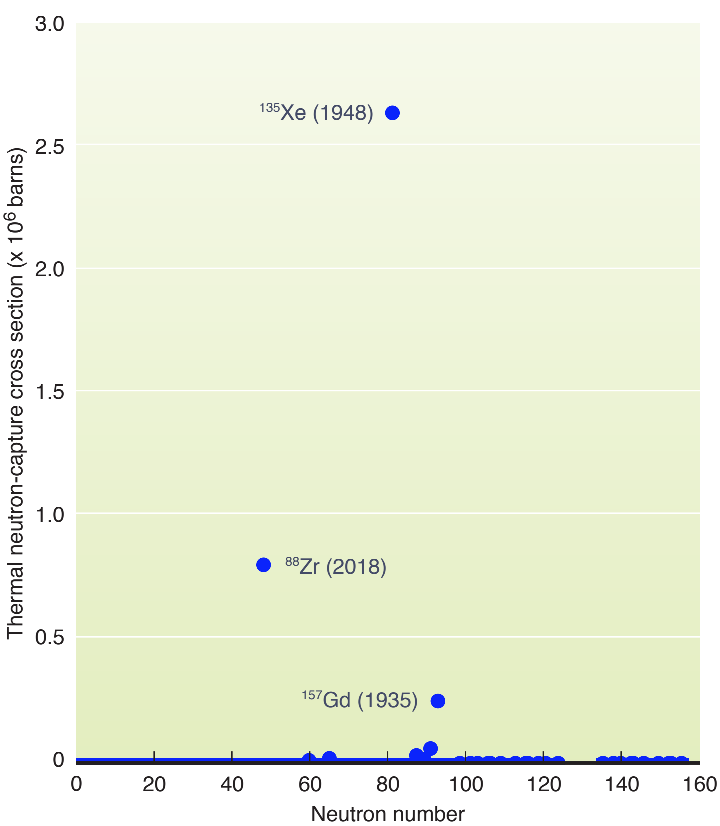
Scientific Serendipity

The team's initial harvesting experiment at NSCL yielded a single, purified, irreplaceable ^{88}Zr target for subsequent cross-section experiments. "Typically, at least 10^{17} atoms are required to create a target that is sufficient for cross-section measurements," says Scielzo. "With stable isotopes, gathering this amount is trivial, but with radioactive isotopes it becomes much harder to amass enough atoms with sufficient purity." With only one chance available at NSCL to conduct cross-section measurements on their harvested ^{88}Zr target, Scielzo and his team turned to the University of Alabama at Birmingham (UAB) to produce practice samples for preliminary tests.

Former Livermore postdoctoral researcher Jennifer Shusterman, played a central role in the project's success by preparing and purifying the samples before and after the tests. (Shusterman is now an assistant professor at Hunter College in New York.) At the UAB Cyclotron Facility, targets were produced by bombarding a high-purity yttrium target with protons. Extensive chemical separation processes and analysis of the irradiated target followed to ensure the purity of the final ^{88}Zr samples, which were then shipped to the University of Missouri's Research Reactor (MURR).

Zirconium-88 has a well-defined gamma-ray signature, which appears at an energy of 393 kiloelectronvolts (keV) following its decay. When ^{88}Zr absorbs another neutron, it becomes zirconium-89 (^{89}Zr), which has its own gamma-ray signature at 909 keV following decay. The distinction between the two signatures makes the neutron-capture transition straightforward to measure. At MURR, the purified samples were bathed in a huge number of low-energy thermal neutrons, which are especially suited for the ^{88}Zr to ^{89}Zr transition. The samples were irradiated for two days, then prepared and shipped to Lawrence Livermore for analysis.

The team expected to record a tiny fraction of the ^{88}Zr atoms transforming into ^{89}Zr using gamma-ray spectroscopy techniques, and then refine their measurements in preparation for the upcoming experiment at NSCL. Based on calculations, Scielzo anticipated the cross section to be about 10 barns—the unit that measures how many atoms undergo neutron capture—so that only about 1 out of every 10,000 ^{88}Zr atoms should be transmuted. Instead, after 48 hours inside MURR, the decay counting back in Livermore seemed to indicate that the ^{88}Zr decay signature had completely disappeared and had been replaced by a strong ^{89}Zr decay signature. In other words, results seem to indicate that almost the entire sample had transformed into ^{89}Zr. "In most experiments, we expect our predictions to be in the right ballpark," says Scielzo. "This time, it appeared we weren't even in the right continent."



Data collected by Lawrence Livermore and its collaborators revealed the second-highest neutron-capture cross section ever observed. The highest neutron-capture cross section was discovered more than 70 years ago and belongs to xenon-135—a short-lived fission product.

When it Doubt, Try, Try Again

In Livermore, nuclear physicists and radiochemists alike were skeptical of the results. "Our first response was to question what had gone wrong," says Scielzo. "We asked ourselves whether it was possible that all the zirconium-88 leaked out somehow, or if the sample could have been contaminated by something else masquerading as zirconium-89." The team knew they had to repeat the experiment to verify the data.

After new material was made at the UAB Cyclotron Facility, the team sent seven identical ^{88}Zr samples back to MURR to be irradiated. The first was removed after 5 minutes, the second after 15 minutes, and the third after an hour. Four more targets were removed at intervals up to 48 hours, and all seven were immediately shipped back to Livermore to be analyzed. Since ^{89}Zr has a half-life of only three days, any delay in shipping would compromise the sample.

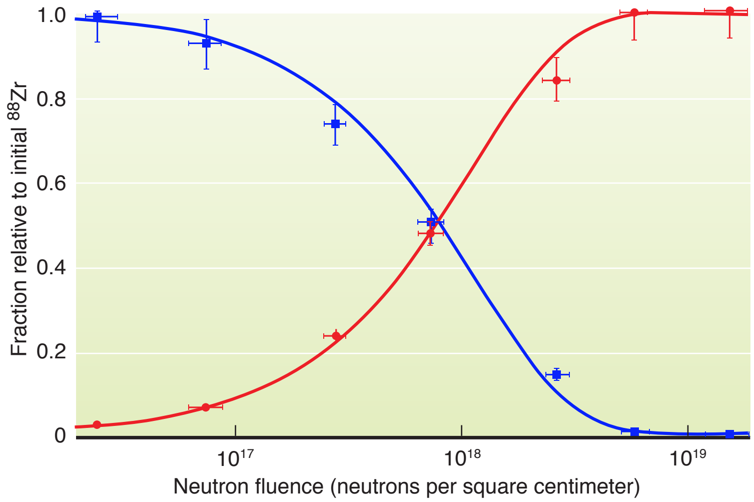
Once again, analysis revealed that the gamma-ray signatures of this second group of samples showed a normal, if extraordinarily productive, progression of neutron-capture reactions transmuting ^{88}Zr to ^{89}Zr. The longer the sample was bombarded with neutrons, the larger the fraction of atoms that were converted. The results confirmed that the cross section was not anywhere near 10 barns, but instead 850,000 barns. Lawrence Livermore and its collaborators had stumbled upon the second-highest neutron-capture cross section ever seen. (The record holder for highest neutron-capture cross section belongs to xenon-135, a short-lived fission product that influences the performance of nuclear reactors.) Says Scielzo, "Through these tests, we confirmed that this unexpectedly high cross section was in fact the result of physics and not just some mistake we made in the experiment."

This work provides yet another example of how multidisciplinary science in action yields fruitful results. Along with Scielzo, Shusterman, and their university colleagues, other Livermore team members include nuclear chemist Dawn Shaughnessy, physicist Keenan Thomas, and nuclear physicist Anton Tonchev. "The overall collaboration between chemists and physicists was pivotal to this project," says Scielzo. "The physicists could not have performed the chemistry work needed to prepare and isolate the ^{88}Zr samples, and the radiochemists benefited from the experience of the physicists in measuring cross sections."

Winning the Nuclear Lottery

Scielzo notes that since the two highest neutron-capture cross sections ever recorded are for radioactive isotopes, many more interesting revelations may come to light as scientists perform experiments with advanced capabilities such as FRIB. Radioactive isotopes are notoriously difficult to study, and this unexpected finding highlights how little is known about the interaction of radioactive isotopes with neutrons. "To have a cross section of this size depends upon finding an isotope with the right nuclear state at exactly the right energy," says Scielzo. "We won the nuclear lottery with zirconium-88."

Recently, the research team conducted its long-awaited experiment on ^{88}Zr at NSCL and began analyzing the results.



The populations of ^{88}Zr (blue squares) and zirconium-89 (^{89}Zr, red circles) as a function of neutron fluence—the total number of neutrons that passed through a unit area—were measured following irradiation of the initial ^{88}Zr sample. The blue and red solid lines show the corresponding fitting curves, from which the neutron-capture cross section was determined. As indicated, with exposure to neutrons, the ^{88}Zr atoms were rapidly transmuted to ^{89}Zr.

With FRIB's imminent completion, the researchers are looking forward to the production and harvest of many exotic, radioactive isotopes and their potential in future applications. According to Scielzo, FRIB offers the opportunity to rectify the long-standing gap in understanding reactions of radioactive nuclei needed to improve our knowledge of the origins of heavy elements and to measure nuclear data required for high confidence in the safety, security, and effectiveness of the U.S. stockpile.

The success of this team is twofold. The researchers effectively demonstrated that enough radioisotopes can be harvested from experiments to create targets for further scientific research and proved the follow-on research could yield significant dividends. Nature still has secrets to reveal, and eager scientists are looking forward to many more surprises.

—Ben Kennedy and Caryn Meissner

Key Words: exotic nuclei, Facility for Rare Isotope Beams (FRIB), gamma-ray spectroscopy, isotope harvesting, ion beam, National Superconducting Cyclotron Laboratory (NSCL), neutron-capture cross section, radioactive isotope, stockpile stewardship, zirconium.

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Patents and Awards

In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven- or eight-digit number in the search box at the U.S. Patent and Trademark Office's website (www.uspto.gov).

Patents

Assessment of Tissue or Lesion Depth Using Temporally Resolved Light Scattering Spectroscopy
Stavros G. Demos
U.S. Patent 10,413,188 B2
September 17, 2019

Capacitive Deionization Charge Transfer from One Capacitor Simultaneously to Multiple Capacitors
Steven L. Hunter, Michael Stadermann
U.S. 10,427,958 B2
October 1, 2019

Modified Cyclodextrins for the Selective Sequestration of Fentanyl-Related Compounds and Uses Thereof
Daniel Joseph Kennedy, Brian P. Mayer, Carlos A. Valdez
U.S. Patent 10,442,871 B2
October 15, 2019

Flexure-Based, Tip-Tilt-Piston Actuation Micro-Array
Jonathan Hopkins, Robert Matthew Panas
U.S. Patent 10,444,492 B2
October 15, 2019

Halbach-Array Radial Stabilizer for a Passive Magnetic Bearing
Richard F. Post
U.S. Patent 10,447,110 B2
October 15, 2019

Awards

Five teams of Livermore researchers and one individual were honored with **Defense Programs Awards of Excellence** from the **National Nuclear Security Administration** (NNSA). The awards honored work performed in 2018 that was critical to ensuring the safety, security, and effectiveness of the nation's nuclear deterrent.

The **Methuselah Team** received the award for developing a simple method for ameliorating the aging process in existing systems and delaying it in future life-extension programs (LEPs). The **Compton Radiography Team** developed and demonstrated an experimental capability at the National Ignition Facility (NIF), which produced the first-ever time-resolved Compton radiograph of an inertial confinement fusion implosion. In honor of exceptional support to an effort known as the 50+10 Study, an **Integrated Project Team**, consisting of personnel from NNSA, Lawrence Livermore, and Y12, received the award for a series of tests they performed from FY16 through FY18 that leveraged NNSA's planned dismantlement of secondaries at the Y12 facility.

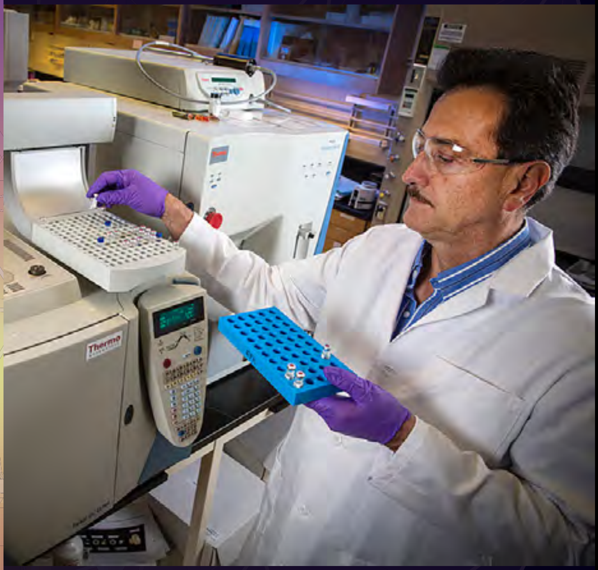
Joseph Kilkenny was recognized for his exceptional contributions to the Stockpile Stewardship Program through his leadership of NNSA's National Diagnostics Initiative (NDI) over the last six years. NDI has led to revolutionary advances in the ability to diagnose the behavior of matter at NNSA's three high-energy-density (HED) experimental facilities. The **LEP Assessment of Replacement Materials Team** used NIF to deliver HED data that enables LEP assessment of replacement material options. These experiments are a continuation of previous HED platform development efforts designed to measure material equation-of-state (EOS) data for a wide range of pressure regimes. In recognition of its contributions to producing a detailed next-generation plutonium (Pu) EOS model for stockpile applications, the **Pu EOS Team** also garnered this prestigious award. The model included new ab initio calculations to constrain the Pu EOS in areas previously lacking such constraints and also incorporated new high-pressure Pu data.

Lawrence Livermore employees **Genaro Mempin**, **Patrick Dempsey**, and **Chris Spadaccini** received a 2019 **"Best in Class" National Technology Transfer Award** from the **Department of Energy's Technology Transfer Working Group** (TTWG) for their efforts to create the Advanced Manufacturing Laboratory (AML). The award was presented in the category of economic development.

Located in the unclassified research area of the Livermore Valley Open Campus, the 14,000-square-foot AML enables Lawrence Livermore to expand collaborative research partnerships with industry, nearby Sandia National Laboratories/California, universities, student researchers, and local businesses. To date, several partnerships have been established with companies in the energy, security, and manufacturing fields.

Inaugurated in 2018, the TTWG awards recognize technology transfer professionals in five categories—intellectual property management, licensing, partnering, economic development, and innovative lab facilities. This year's award marks the second straight year that the Laboratory has won a TTWG "Best in Class" honor.

The Effort to Ban Chemical Weapons



The Forensic Science Center develops novel analytical methods and trains at-risk nations to respond to incidents involving toxic chemicals.

Also in August

- *The Laboratory's fastest supercomputer runs mission-driven simulations on specially optimized hardware and software.*
- *Working in a mile-deep tunnel, researchers are learning how to turn heat from dry rock into clean, low-carbon-emitting power.*
- *A promising manufacturing method applies tiny droplets of molten metal layer by layer.*

Coming Next Issue

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